

Model Performance

Model	Data
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Weighted KNN model					
5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.87	0.81	0.87	0.82	0.86	0.86

## Model Results

**Predicted value:** 5.11 mol/L

**Global applicability domain:** Inside

**Local applicability domain index:** 8.05e-01

**Confidence level:** 6.55e-01

## Nearest Neighbors from the Training Set

Image not found

Acrolein

**Measured:** 3.78

**Predicted:** 5.11

Image not found

Acetaldehyde

**Measured:** 22.7

**Predicted:** 13.1

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Acetone

**Measured:** 17.2

**Predicted:** 6.59

Image not found

Methacrylaldehyde

**Measured:** 8.08e-01

**Predicted:** 2.22

Image not found

Propanal

**Measured:** 5.27

**Predicted:** 3.91